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Account of Non-Diagonal *d-d*-Electron Couplings in Fe-Co Liquid Alloy

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Abstract

The partial Wills-Harrison effective pair potentials in liquid equiatomic Fe-Co alloy are considered. It is shown that the account of the non-diagonal *d-d* couplings between electrons leads to the same changes in characteristics of the pair-potential first minimum as in the case of the pure transition metals.

Keywords: liquid Fe-Co alloy, transition metal, Wills-Harrison model, *d*-state coupling

The Wills-Harrison [1] partial effective pair potentials, $\varphi_{ij\mathrm{WH}}(r)$, between atoms Fe and Co in equiatomic Fe-Co alloy at *T*=1863K are calculated at different values of the suggested in [2] probability *p* that not only diagonal *d-d* couplings are possible at condition that all *d-d* couplings (diagonal and non-diagonal) are equiprobable in this case.

Following [3] we use the local Bretonnet-Silbert (BS) model pseudopotential [4] extended to binary alloys in [5] for description the *s*-electron contribution, $\varphi_{sij}(r)$, to $\varphi_{ij\mathrm{WH}}(r)$.

As follows from the previous paper, $\varphi_{ij\mathrm{WH}}(r) = \varphi_{sij}(r)$ at $p = 1$. It denotes here that $\varphi_{ij\mathrm{WH}}(r) = \varphi_{ij\mathrm{BS}}(r)$ at $p = 1$.

It is clear from Fig.1 that changing *p* from 0 up to 0.5 slightly influences the depth and position of the first minimum of $\varphi_{ij\mathrm{WH}}(r)$. At the same time, these characteristics become strong different at $p = 1$. Such a tendency is the same as it

was observed in the case of pure transition metals [2].

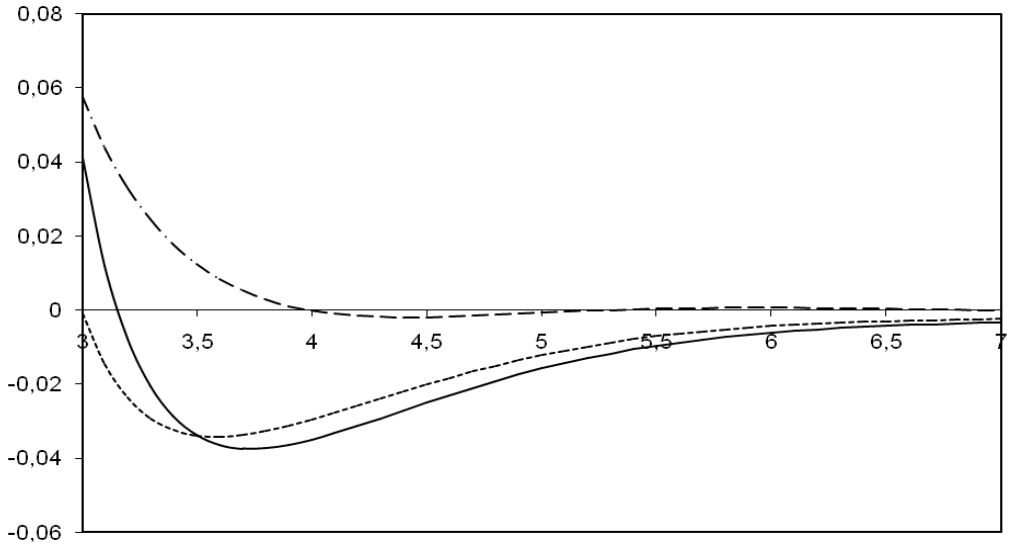

Figure 1. $\varphi_{ij\mathrm{WH}}(r)$ between atoms Fe and Co in liquid equiatomic Fe-Co alloy ($p = 0$ – solid line; $p = 0.5$ – dotted line; $p = 1$ – dashed-dotted line).

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